Interfacial strain in $Al_xGa_{1-x}As$ layers on GaAs

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Detailed analysis of x-ray rocking curves was used to determine the depth profile of strain and composition in a 2500-Å-thick layer of $Al_xGa_{1-x}As$ grown by metalorganic chemical vapor deposition on ⟨100⟩ GaAs. The x value and layer thickness were in good agreement with the values expected from growth parameters. The presence of a transition region, 280 Å thick, was detected by the rocking curve. In this region, the Al concentration varies smoothly from 0 to 0.87. Measurement and control of the sharpness of such interfaces has important implications for heterojunction devices.

In epitaxially grown layers where the composition is modulated, one expects the existence of interfacial transition regions with smoothly varying composition. It is difficult to predict from first principles or growth conditions the thickness of such a region. Measurement of transition regions is also difficult. The x-ray rocking curve has been shown[1-3] to be a highly sensitive tool for measuring strains due to composition variations. More recently the technique has also been used to obtain detailed strain profiles in epitaxial structures.[3-5] In this letter, we report rocking curve measurements which demonstrate that the technique can probe transition regions with thicknesses above ~50 Å.

The $Al_xGa_{1-x}As$ layers used in this study were grown by metalorganic chemical vapor deposition (MOCVD) on GaAs substrates oriented 2° to 3° off ⟨100⟩ axis. The layers were grown in a computer-controlled reactor at ~730 °C. The trimethylaluminum and trimethylgallium ratios to arsene were adjusted to obtain a growth rate of ~550 Å/min. From the growth parameters, the expected Al concentration was ~0.88 and the layer thicknesses ~2200 Å. Bragg case double-crystal x-ray rocking curves were obtained with the $FeK_{\alpha 1}$ (400) reflection. The x-ray beam was collimated and rendered nearly monochromatic by (400) reflection in ⟨100⟩ GaAs. The incident beam divergence was below 20 arcsec. The spot size was limited to ~2 mm × 1 mm. Experimental rocking curves were fitted using the method of Ref. 4. For the calculated curves, a structure factor and absorption coefficient in the epitaxial layer corresponding to 0.88 Al was used. The strain profiles obtained are in the direction perpendicular to the surface and with respect to the GaAs substrate.

Figure 1(a) shows experimental (dashed line) and calcu-

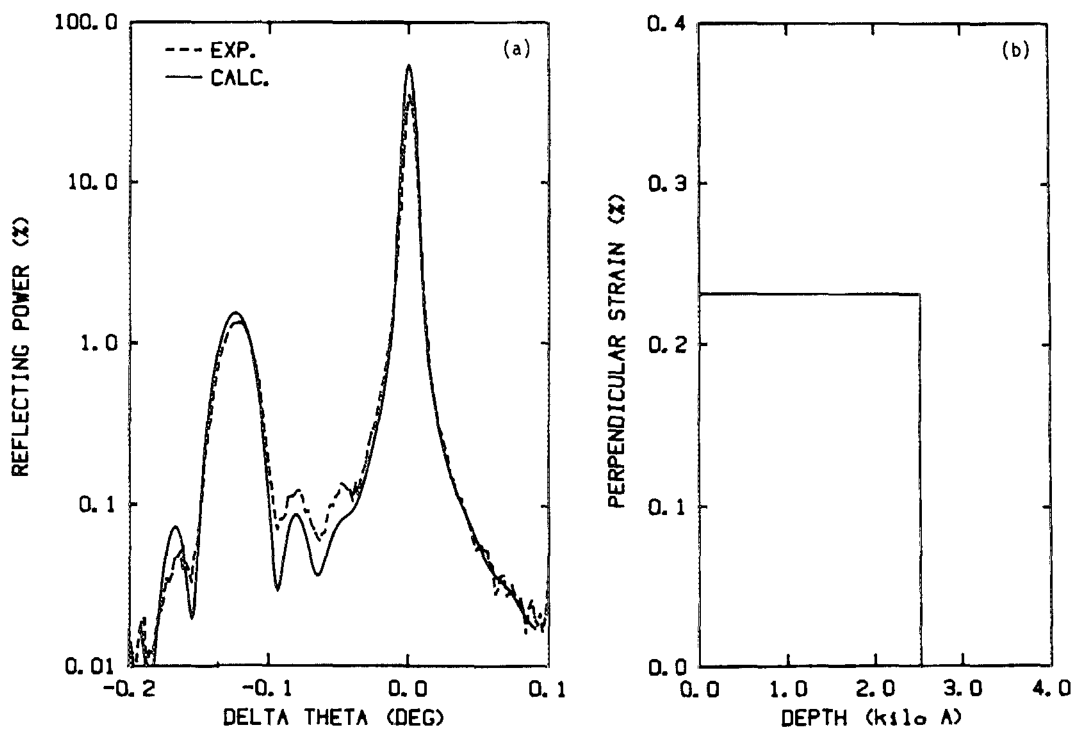

FIG. 1. (a) Measured (dashed line) and calculated (solid line) $FeK_{\alpha 1}$ (400) x-ray rocking curves of a $Al_xGa_{1-x}As$/GaAs sample. The calculated curve corresponds to the flat strain profile shown in (b).

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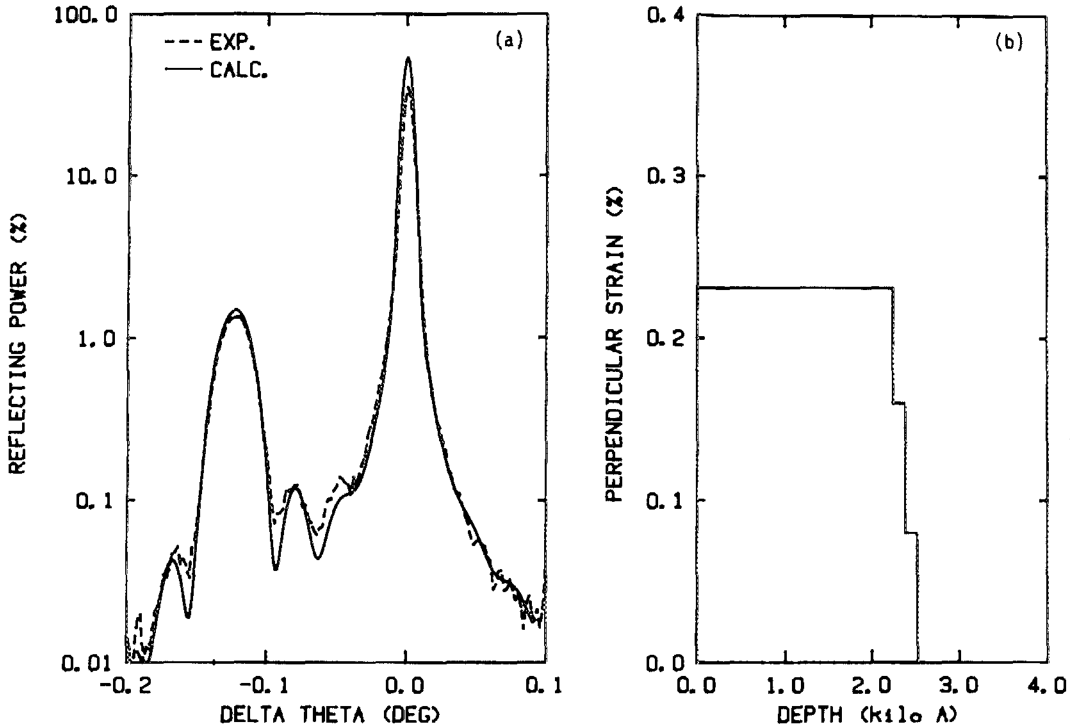

FIG. 2. (a) Measured (dashed line) and calculated (solid line) Fe$K_{\alpha 1}$ (400) x-ray rocking curves of the same sample as in Fig. 1. The calculated curve in this case includes a 280-Å thick transition region with strain profile as shown in (b).

ed (solid line) rocking curves of a representative sample. The angle $\Delta\theta$ is plotted relative to the Bragg angle of the substrate peak, which has a maximum reflecting power of $\sim 50\%$. The oscillatory structure at $\Delta\theta < 0$ is due to the epitaxial layer. The calculated curve is obtained from the strain profile of Fig. 1(b). The strain $\epsilon^{\perp} = 0.231\%$ and the thickness $T = 2520$ Å produce a reasonably good fit to the experimental curve [Fig. 1(a)]. However, there remains a discrepancy between measured and calculated amplitudes of the subsidiary oscillations, especially for $-0.1° < \Delta\theta < -0.03°$. This discrepancy can only be removed [Fig. 2(a)] by a strain profile which includes a transition region, as shown in Fig. 2(b). The thickness (280 Å) of this region and its strain profile are determined by matching the experimental curve.

An increase of 140 Å in the thickness of the transition region [Fig. 3(b)] results in a distinctly poorer fit [Fig. 3(a)]. Comparison of Figs. 1 through 3 clearly demonstrates the sensitivity of the technique in detecting the transition region

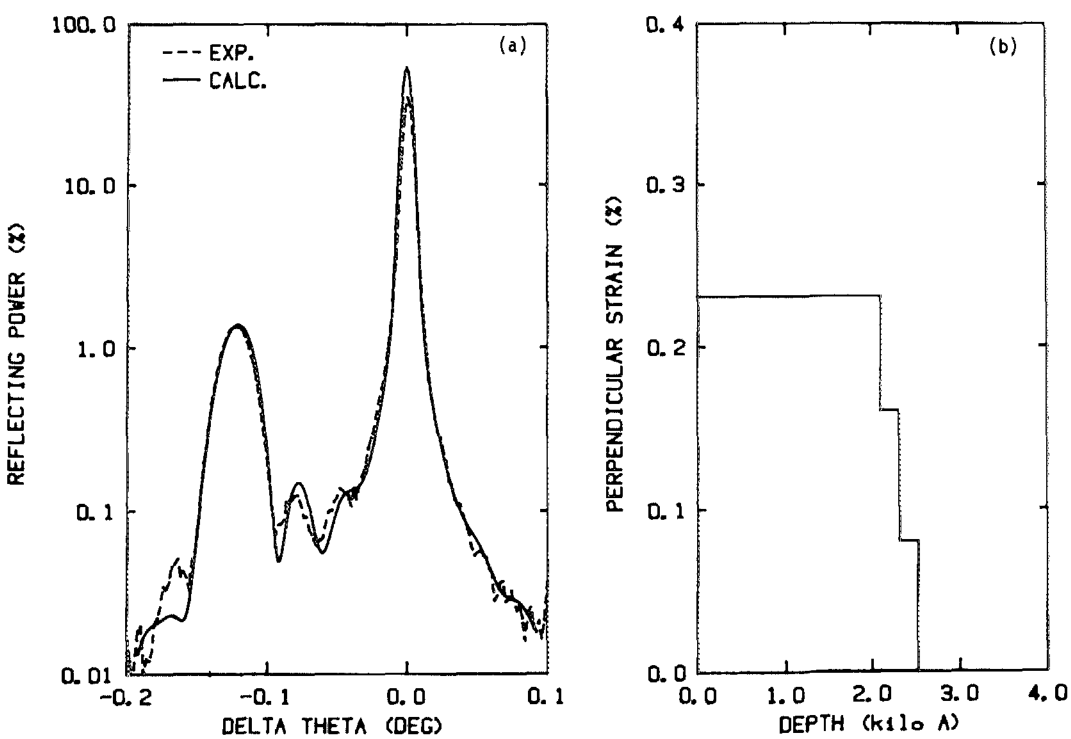

FIG. 3. (a) Measured (dashed line) and calculated (solid line) Fe$K_{\alpha 1}$ (400) x-ray rocking curves of the same sample as in Fig. 1. The calculated curve corresponds to the strain profile in (b) with a 420-Å transition region.

and also in determining its thickness. The thickness is 280 Å to an accuracy better than 50 Å. Although the strain is expected to vary smoothly, its profile in this region is represented by two discrete, equally spaced steps since the resolution does not permit finer detail. Due to the very low absorption of x rays in thin layers, the calculated curve is insensitive to mirror reflections of the strain profile. Thus the transition region could be at the air-film interface. In addition, because of the small thickness of the transition region compared to that of the film, the possibility of thinner transition regions on both sides of the film with total thickness of 280 Å cannot be ruled out. This ambiguity can be resolved by etching a few hundred Å off the surface and remeasuring. Independently, the growth conditions suggest that there is only one transition region located at the layer/substrate interface.

From Fig. 2(b), the total thickness of the epitaxial layer is 2520 ± 50 Å. Using bulk AlAs and GaAs lattice parameters and elastic constants of GaAs,[6] a strain $\epsilon^{\perp} = 0.231\%$ corresponds to an Al concentration $x = 0.87$, in good agreement with the expected value (0.88). Since the strain is uniquely related to the concentration of Al, a strain profile corresponds to a profile of Al concentration. Thus the concentration of Al varies smoothly from 0 to 0.87 over a 280-Å-thick transition region at the layer/substrate interface.

In conclusion, the x-ray rocking curve technique is an excellent tool for the characterization of interfacial transition regions. For the epitaxial $Al_xGa_{1-x}As$ layer, 2520 Å thick, considered in this letter, the thickness of the transition region has been measured with an accuracy better than 50 Å.

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